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A decorated Ising model for DYE-DNA interactions

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The interactions between aminoacridine dyes and DNA involve two types of binding sites and two modes of binding, one with higher energy considered as intercalation process, the other with lower energy due to external binding of the dye molecules with the phosphate groups of DNA. Moreover, the binding is expected to involve some base specificity. Theoretical studies undertaken so far have been worked out mostly from a combinatorial point of view with the binding sites playing the role of holes in which the dye molecules can be placed. The intermolecular ingeractions have been incorporated as a statistical weight factor (Blake & Peacocke 1968, Bradley & Lifson 1968, Schwarz 1970, Hill 1960, Armstrong *et al* 1970). However the problem of excluded site and base specificity has not been explained. The adsorption isotherm for dye-DNA systems exhibit two broad regions (figure 1a) (Peacocke & Skerrett 1956), one at low dye concentration representing intercalative binding and the other, dominating at higher dye concentration, represents the weaker external binding. The binding isotherm is of Langmuir type (figure 1b) (Waring 1965) for dyes in which the external

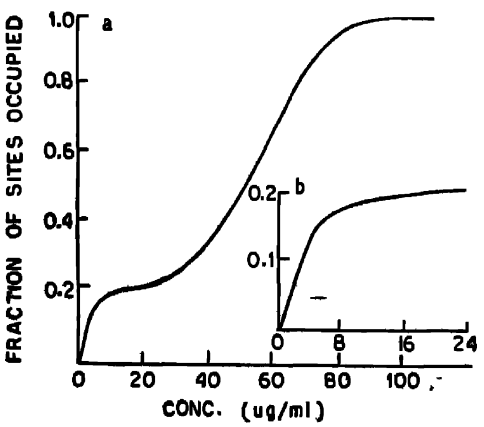

Fig. 1. Typical binding isotherms.
(a) DNA-proflavine complex. (Peacock & Skerrett 1956)
(b) DNA-ethidium bromide (Waring 1965)

binding is relatively insignificant. It has been suggested that each binding site can accommodate more than one dye molecule (Armstrong *et al* 1970, Fredrieq & Houssier 1972).

The purpose of the present report is to propose a model for the dye-DNA interaction in terms of a decorated Ising lattice in which the base-pairs form the decoration lattice in which the intercalation and phosphate binding sites are embedded. The base pair sites (i-sites) are coupled with the sites for the two types of binding (j and k sites) i.e., the dye molecules in j and k sites interact indirectly with each other through the intervention of base pairs (superexchange). The AT and GC base pairs are represented by the Ising dicotomic variable σ_i. For the j and k sites the Ising variables are μ_j and ρ_k respectively, each having eigenvalues 0, ± 1. Zero signifies no occupancy of a binding site and the value ± 1 are associated with two types of binding for each type of site j and k. To each configuration $\{\sigma_i, \mu_j, \rho_k\}$ we may associate (assuming nearest neighbour interaction) the Hamiltonian (H)

$$H = \frac{J}{2} \sum_{<i,j>} \sigma_i \mu_j + \frac{J'}{2} \sum_{<i,k>} \sigma_i \rho_k - \lambda c(\Sigma \mu_j + \Sigma \rho_k) + K[\Sigma(\mu_j)^2 + \Sigma(\rho_k)^2], \quad \ldots (1)$$

where c is the concentration of the dye molecules, λ is related to the absolute activity of the free dye and K is the chemical potential of bound dyes. J and J' are interaction parameters to be determined emperically. The symbols $<i, j>$ and $<i, k>$ means that the summation should be taken over only the nearest neighbour sites.

The grand partition function for the system can be written as

$$\Xi = Tr\,[\exp(-H/k_B T)] \quad \ldots (2)$$

where k_B and T are Boltzman constant and temperature respectively. Using the well known decoration transformation (Fisher 1960) the grand partition function can be reduced to the factored form

$$\Xi = f^{2N} Q \quad \ldots (3)$$

where $2N$ is the total number of available sites, Q is the cononical partition function of the undecorated lattice and f is a factor depending on the base pair lattice.

Detailed computation of thermodynamic parameters is in progress. However, it is interesting to discuss certain phase diagrams presented by Masiyama & Nara (1973), for the corresponding decorated Ising treatment for magnetic phase transition (shown schematically in figure 2). It may be pointed out that magnetisation and magnetic field for the magnetic Ising system corresponds to the fraction of bound dyes and free dye concentration respectively in the present problem. Depending on the strength and nature of the dye-DNA interaction

parameter one has the different shaped isotherms (figure 1) which in the corresponding magnetic case is shown explicitly by Mashiyama & Nara (1973) by varying the interaction parameter involved in the phase diagram computation. The excluded site problem is also explained by the first saturation level occuring at $m = 0.2$ which is also the value for the corresponding binding isotherm.

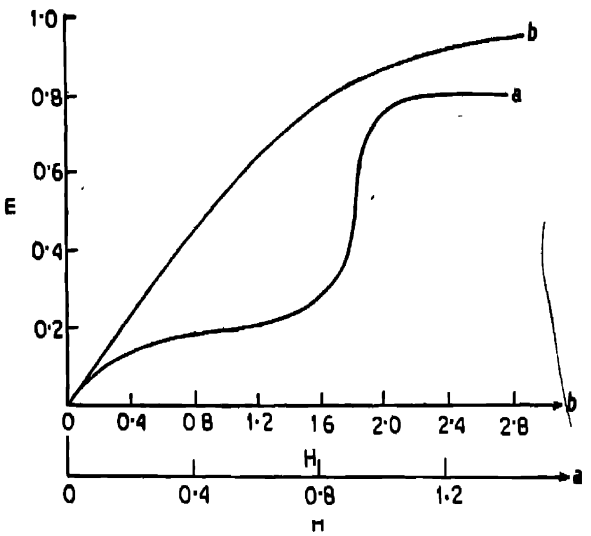

Fig. 2. The magnetisation curves as function of magnetic field for different values of dilution parameter and magnetic ion concentration(Masiyama & Nara 1973)

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